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QUANTUM AND EXCHANGE CORRECTIONS TO PLASMA KINETIC THEORY*

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ABSTRACT

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By means of a quantum-mechanical phase space distribution function introduced by von Roos, the Schroedinger equation appropriate to a plasma can be transformed into a quantum mechanical generalization of the Liouville equation. From the consequent analog of the BBGKY hierarchy, the two-electron correlation function in a spatially homogeneous fully ionized plasma is obtained by assuming that the ions can be treated as an immobile uniformly charged background. The resulting equation for the electron distribution function is a quantum mechanical Boltzmann equation, whose collision integral differs from that derived by Balescu and others in that exchange effects are more properly taken into account. In particular, a new term appears in the collision integral which is identifiable with the Mott correction to electron-electron scattering, and is shielded by the dynamical dielectric constant of the plasma in a somewhat unexpected fashion. A consequence of this term is an alteration of the large momentum transfer contribtuions to the collision integral appropriate to a "classical" plasma.

A central problem in the description of non-equilibrium phenomena in classical plasmas is that of obtaining from the N-particle Liouville equation a kinetic (or "Boltzmann") equation for the single-particle phase space distribution function. Proceeding along different lines, several investigators[1-4] have derived a kinetic equation valid in the limit where the number of particles in a Debye sphere is large compared to unity.

For the particular case* of an electron plasma in a uniform background of neutralizing positive charge and no magnetic field, one obtains the coupled equations

$$\left[\frac{\partial}{\partial t} + \underset{\sim}{v}\cdot\nabla_{\underset{\sim}{x}} - \frac{e}{m}\left(\underset{\sim}{E}^{ext}(\underset{\sim}{x},t) + \underset{\sim}{E}^{SCF}(\underset{\sim}{x},t)\right)\cdot\nabla_{\underset{\sim}{v}}\right]f(\underset{\sim}{x},\underset{\sim}{v},t) = \left(\frac{\partial f}{\partial t}\right)_{Coll.} \qquad (1)$$

$$\underset{\sim}{\nabla}\cdot\underset{\sim}{E}^{SCF}(\underset{\sim}{x},t) = -4\pi e n\left[C\int d^3v\, f(\underset{\sim}{x},\underset{\sim}{v},t) - 1\right] \qquad (2)$$

$$\left(\frac{\partial f}{\partial t}\right)_{Coll.} = \frac{2ne^4}{m^2}C\,\nabla_{\underset{\sim}{v}}\int d^3v'\left\{\int d^3q\,\frac{\underset{\sim}{q}\,\underset{\sim}{q}}{q^4}\,\frac{\delta\left(\underset{\sim}{q}\cdot(\underset{\sim}{v}-\underset{\sim}{v}')\right)}{\left|K(\underset{\sim}{q},\underset{\sim}{q}\cdot\underset{\sim}{v})\right|^2}\right\}$$

$$\cdot\left\{\left(\nabla_{\underset{\sim}{v}} f(\underset{\sim}{v})\right)f(\underset{\sim}{v}') - f(\underset{\sim}{v})\left(\nabla_{\underset{\sim}{v}'} f(\underset{\sim}{v}')\right)\right\} \qquad (3)$$

Equation (1) is the kinetic equation, in which electron-electron interactions enter both through the self-consistent electric field, E^{SCF}, and through the "collision integral," representing the effect of fluctuations of the electric field about this value. Equation (2) is Poisson's

*In the interest of simplicity, the considerations of this paper will be limited to this case. The extension of the method to include ionic degrees of freedom and external magnetic fields is relatively straightforward and will be published elsewhere.

equation for the self-consistent field, n being the average electron (and ion) number density. The third equation gives the specific form of the collision integral which is seen to depend on the dynamic dielectric constant of the plasma, as given by the expression

$$K(\underset{\sim}{q},\omega) = 1 + \frac{\omega_p^2}{q^2} C \int d^3v \, \frac{\underset{\sim}{q} \cdot \nabla_{\underset{\sim}{v}} f(\underset{\sim}{v})}{\omega + i\epsilon - \underset{\sim}{q} \cdot \underset{\sim}{v}} \tag{4}$$

where $\omega_p^2 = 4\pi n e^2/m$ is the plasma frequency squared and ϵ is a positive infinitesimal. The constant C appearing in (2) - (4) is determined by the normalization of the single-electron distribution function, f, and is unity for the particular choice

$$\int d^3x \int d^3v \; f(\underset{\sim}{x},\underset{\sim}{v},t) = V \tag{5}$$

where V is the volume of the system (a convention we will generally follow unless otherwise indicated).

The quantum mechanical generalization of these equations is of some interest, both for the purpose of extending the classical kinetic theory of plasmas to those regimes of density and temperature where quantum effects must be considered, as well to provide a description of intrinsically quantum mechanical systems (e.g. the electron gas in a metal) which makes more extensive use of classical concepts than the widely prevalent alternative formulations based on quantum field theory. Although our present concern is clearly limited to the first of these objectives, it is worth noting in passing that the kinetic theory of quantum plasmas on which this paper is based appears[5] to be a promising approach to the general quantum many-body problem.

The first definitive extension of equations (1) - (4) to quantum plasmas is apparently that of Balescu[6]. Basically similar subsequent studies by Silin[7] and Guernsey[8] may also be cited. In essence, these investigations proceed from Wigner's[9] observation that by shifting attention from the wave function of a many-particle system to a quantum-mechanical phase space distribution function (q.m.d.f.) derived therefrom, it is possible to formulate the quantum statistical mechanics of interacting systems (i.e. plasmas) in a fashion which bears a close resemblance to the classical theory. Indeed, the q.m.d.f. obeys an equation which is a quantum generalization of the Liouville equation and, in fact, becomes identical to the Liouville equation in the limit $\hbar \to 0$. Then, by proceeding in strict analogy to the so-called BBGKY approximation scheme which, in the classical situation, leads from the Liouville equation to the Vlasov Theory in first approximation, and to equations (1) - (4) in the second, one generates a corresponding kinetic theory of quantum plasmas.

The quantum generalization of the collision integral (equation (3)) which results from this program may be written in the form

$$\left(\frac{\partial \tilde{f}(\underset{\sim}{v})}{\partial t}\right)_{\text{coll.}} = -\frac{4 n e^4}{\hbar^2}\int d^3v' \int d^3q\, \frac{1}{q^4}\, \frac{1}{|\tilde{K}(\underset{\sim}{q}, \underset{\sim}{q}\cdot\underset{\sim}{v})|^2}\, \delta\!\left(\underset{\sim}{q}\cdot(\underset{\sim}{v}-\underset{\sim}{v}') + \frac{\hbar q^2}{m}\right)$$

$$\times \left\{ \tilde{f}(\underset{\sim}{v})\tilde{f}(\underset{\sim}{v}')\left[1 - \frac{nh^3}{2m^3}\tilde{f}\left(\underset{\sim}{v}+\frac{\hbar}{m}\underset{\sim}{q}\right)\right]\left[1 - \frac{nh^3}{2m^3}\tilde{f}\left(\underset{\sim}{v}'-\frac{\hbar}{m}\underset{\sim}{q}\right)\right]\right.$$

$$\left. - \tilde{f}\left(\underset{\sim}{v}+\frac{\hbar}{m}\underset{\sim}{q}\right)\tilde{f}\left(\underset{\sim}{v}'-\frac{\hbar}{m}\underset{\sim}{q}\right)\left[1 - \frac{nh^3}{2m^3}\tilde{f}(\underset{\sim}{v})\right]\left[1 - \frac{nh^3}{2m^3}\tilde{f}(\underset{\sim}{v}')\right]\right\} \qquad (6)$$

where the tildes serve to distinguish quantum-corrected quantities from those introduced earlier.

The dielectric constant appearing in (6) is the quantum generalization of (4) and is usually referred to in the literature as the RPA ("random phase approximation") dielectric constant. It is given by the expression

$$\tilde{K}(\underset{\sim}{q},\omega) = 1 + \frac{\omega_p^2}{q^2}\frac{m}{\hbar}\int d^3v \, \frac{\tilde{f}(\underset{\sim}{v}+\frac{\hbar}{m}\underset{\sim}{q}) - \tilde{f}(\underset{\sim}{v})}{\omega + i\epsilon - \underset{\sim}{q}\cdot\underset{\sim}{v} - \frac{\hbar q^2}{2m}} \tag{7}$$

In the limit $\hbar \longrightarrow 0$, $\tilde{K} \longrightarrow K$, $\tilde{f} \longrightarrow f$, and (3) is readily recovered from (6).

The physical significance of equation (6) has been clarified by the observation of Wyld and Pines[10], that it could have been written down immediately using the "golden rule" of scattering theory, if one makes the plausible conjecture that the Coulomb scattering matrix element should be augmented by the dynamical dielectric constant of the plasma. Specifically, if one takes as the matrix element for the scattering of two electrons from (wave-vector) states $\underset{\sim}{p}, \underset{\sim}{p}'$ to states $(\underset{\sim}{p}+\underset{\sim}{q}), (\underset{\sim}{p}'-\underset{\sim}{q})$ the quantity

$$\langle \underset{\sim}{p}+\underset{\sim}{q}, \underset{\sim}{p}'-\underset{\sim}{q} | S | \underset{\sim}{p}, \underset{\sim}{p}' \rangle = \frac{1}{V}\frac{4\pi e^2}{q^2}\left[\tilde{K}(\underset{\sim}{q}, \hbar^{-1}(\epsilon_{p+q} - \epsilon_p))\right]^{-1} \tag{8}$$

where $\epsilon_p \equiv \hbar^2 p^2/2m$, then the "golden rule" for the transition probability per unit time of this process:

$$\frac{2\pi}{\hbar}\left|\langle \underset{\sim}{p}+\underset{\sim}{q}, \underset{\sim}{p}'-\underset{\sim}{q} | S | \underset{\sim}{p}, \underset{\sim}{p}' \rangle\right|^2 \delta(\epsilon_{p+q} + \epsilon_{p'-q} - \epsilon_p - \epsilon_{p'}) \tag{9}$$

leads directly to (6) when the appropriate density of states is introduced.

Viewed in the foregoing light, a deficiency of the collision integral given by equation (6) is immediately apparent. For as is well known, the total cross-section for electron-electron scattering contains contributions from direct Coulomb scattering, exchange scattering, and the interference between these two processes (the so-called "Mott" term). Ignoring for the moment the influence of the dielectric properties of the plasma, one finds that when exchange is included, the (spin-averaged) matrix element appearing in (9) is given in Born approximation by

$$|\langle \underset{\sim}{p}+\underset{\sim}{q}, \underset{\sim}{p}'-\underset{\sim}{q}|S|\underset{\sim}{p},\underset{\sim}{p}'\rangle|^2 = \left(\frac{4\pi e^2}{V}\right)^2\left[\frac{3}{4}\left(\frac{1}{q^2}-\frac{1}{(\underset{\sim}{p}-\underset{\sim}{p}'+\underset{\sim}{q})^2}\right)^2 + \frac{1}{4}\left(\frac{1}{q^2}+\frac{1}{(\underset{\sim}{p}-\underset{\sim}{p}'+\underset{\sim}{q})^2}\right)^2\right] = \left(\frac{4\pi e^2}{V}\right)^2\left\{\frac{1}{q^4}+\frac{1}{(\underset{\sim}{p}-\underset{\sim}{p}'+\underset{\sim}{q})^4}-\frac{1}{q^2(\underset{\sim}{p}-\underset{\sim}{p}'+\underset{\sim}{q})^2}\right\} \tag{10}$$

By symmetry, the first two terms in the curly bracket of (10) would contribute equally to the collision integral, so one would expect the $1/q^4$ factor in (6) to be replaced by (in the limit $\breve{K}\rightarrow 1$)

$$\left[\frac{1}{q^4}-\frac{1}{2q^2\left(\underset{\sim}{q}+\frac{m}{\hbar}(\underset{\sim}{v}-\underset{\sim}{v}')\right)^2}\right] \tag{11}$$

where the additional term represents the Mott correction. We cannot simply add such a correction to (6), however, since it is by no means apparent in what fashion the dielectric properties of the plasma will modify this term.

The absence from equation (6) of the term just cited is a consequence of the well-known inability of the Wigner q.m.d.f. formalism to fully incorporate exchange effects in a tractable fashion. For this reason, increasing use has been made in recent years of an alternative formulation due to von Roos[11]. Employing a somewhat different definition for the q.m.d.f., he is again led to a quantum generalization of the Liouville equation which, however, enables exchange effects to be included in a natural manner. In this paper, therefore, we wish to report the results of a program quite similar to those leading to equation (6) (particularly that of Guernsey[8]) but differing in that the von Roos form of the quantum Liouville equation is used. In essence, the point of departure is that the collision integral thus obtained represents a correction to the Hartree-Fock self-consistent field whereas that obtained in the Wigner formalism represents a correction to the Hartree s.c.f. including, however, enough of exchange to introduce the $\left[1 - \frac{n h^3}{2 m^3}\tilde{f}\right]$ factors in (6) characteristic of the exclusion principle.

The details of the calculation are too lengthy to discuss in the limited time and space available here and will be published elsewhere. Simply stated, we work with the first two equations of the quantum BBGKY hierarchy for the "reduced" q.m.d.f.'s. The first of these couples the singlet and doublet distributions; the second, the doublet and triplet. The doublet distribution function is then written as the properly symmetrized product of singlet functions which one obtains in the Hartree-Fock approximation, plus an unknown two-particle correlation function. The triplet function is similarly decomposed into its Hartree-Fock expression plus cyclical products of singlet and two-particle correlation functions. The coupled equations are thus closed, and one first obtains a solution for the correlation function expressed in terms of the singlet distribution. Insertion of this expression into the first BBGKY equation yields the desired kinetic equation for the singlet function.

We obtain in this fashion the following kinetic equation

$$\left\{ \frac{\partial \tilde{f}}{\partial t} + \underset{\sim}{v} \cdot \nabla_{\underset{\sim}{x}} \tilde{f} - \frac{i\hbar}{2m} \nabla_x^2 \tilde{f} + \frac{ie}{\hbar (2\pi)^3} \int d^3 q \, e^{i \underset{\sim}{q} \cdot \underset{\sim}{x}} \left[\phi^{ext}(\underset{\sim}{q},t) + \phi^{SCF}(\underset{\sim}{q},t) \right] \right.$$

$$\times \left[\tilde{f}(\underset{\sim}{x}, \underset{\sim}{v} + \frac{\hbar}{m} \underset{\sim}{q}, t) - \tilde{f}(\underset{\sim}{x}, \underset{\sim}{v}, t) \right] + \frac{ie^2 \hbar}{(2\pi)^2 \hbar} \int d^3 x' \int d^3 v' \int \frac{d^3 q}{q^2} \, e^{-\frac{im}{\hbar} (\underset{\sim}{v} - \underset{\sim}{v}') \cdot (\underset{\sim}{x} - \underset{\sim}{x}')}$$

$$\left. \times \tilde{f}(\underset{\sim}{x}, \underset{\sim}{v}', t) \left[\tilde{f}(\underset{\sim}{x}', \underset{\sim}{v} + \frac{\hbar}{m} \underset{\sim}{q}, t) - e^{i \underset{\sim}{q} \cdot (\underset{\sim}{x} - \underset{\sim}{x}')} \tilde{f}(\underset{\sim}{x}', \underset{\sim}{v}, t) \right] \right\} = \left(\frac{\partial \tilde{f}}{\partial t} \right)_{Coll.} \qquad (12)$$

The left hand side of (12) is the quantum and exchange corrected Vlasov equation which has been discussed elsewhere[(11)]. In it, we have employed the Fourier transforms of the external and self-consistent potentials which are related to the corresponding electric fields by

$$\underset{\sim}{E}(\underset{\sim}{x},t) = -\underset{\sim}{\nabla}_x \, (2\pi)^{-3} \int d^3 q \, e^{i \underset{\sim}{q} \cdot \underset{\sim}{x}} \phi(\underset{\sim}{q},t) \qquad (13)$$

The self-consistent field is naturally still given by (2). For the collision integral, we obtain in place of (6) the expression

$$\left(\frac{\partial \tilde{f}}{\partial t}\right)_{Coll.} = -\frac{4ne^4}{\hbar^2}\int d^3v' \int d^3q \left[\frac{1}{q^4 |\tilde{K}(\underset{\sim}{q}, \underset{\sim}{q}\cdot\underset{\sim}{v})|^2} - \frac{Re\left([\tilde{K}(\underset{\sim}{q}, \underset{\sim}{q}\cdot\underset{\sim}{v})]^{-1}\right)}{2q^2(\underset{\sim}{q} + \frac{m}{\hbar}(\underset{\sim}{v}-\underset{\sim}{v}'))^2}\right]$$

$$\times\, \delta\left(\underset{\sim}{q}\cdot(\underset{\sim}{v}-\underset{\sim}{v}') + \frac{\hbar q^2}{m}\right) \left\{ \tilde{f}(\underset{\sim}{v})\, \tilde{f}(\underset{\sim}{v}') \left[1 - \frac{nh^3}{2m^3}\tilde{f}(\underset{\sim}{v} + \tfrac{\hbar}{m}\underset{\sim}{q})\right]\left[1 - \frac{nh^3}{2m^3}\tilde{f}(\underset{\sim}{v}' - \tfrac{\hbar}{m}\underset{\sim}{q})\right]\right.$$

$$\left. - \tilde{f}(\underset{\sim}{v} + \tfrac{\hbar}{m}\underset{\sim}{q})\, \tilde{f}(\underset{\sim}{v}' - \tfrac{\hbar}{m}\underset{\sim}{q}) \left[1 - \frac{nh^3}{2m^3}\tilde{f}(\underset{\sim}{v})\right]\left[1 - \frac{nh^3}{2m^3}\tilde{f}(\underset{\sim}{v}')\right]\right\} \tag{14}$$

Comparing (14) and (6), we note that the only difference is in the appearance of the "Mott" term anticipated earlier. The curious result that it is shielded by the real part of K^{-1} rather than $|K|^{-2}$ is unexpected and not understood. In this regard, we remark that in deriving (14), additional terms were obtained which are readily identifiable as <u>three-body</u> collision processes, in which the direct coulomb scattering of two electrons is accompanied by a <u>virtual</u> exchange scattering of one of them with a third electron. We have not included such terms in (14) because other three-body contributions would enter when a higher-order truncation of the BBGKY chain is performed. The possibility that a more exact treatment of three-body and higher correlations would introduce terms into the collision integral which effectively alter the shielding of the Mott term must nevertheless be recognized.

A few remarks concerning (14) are in order. First, it is easily shown that the H-theorem is satisfied so that the collision integral vanishes for the Fermi-Dirac distribution. Due to the presence of the

Mott term, however, the uniqueness of this distribution is by no means apparent. Second, it must be emphasized that (14) is only valid for quasi-homogeneous plasmas in which appreciable density changes occur over distances large compared to the "mean-free path" (and times large compared to the "collision time"), just as in the classical case.

Finally, we note that a straight-forward expansion of (14) in powers of $\hbar$ leads again to (3) in the classical limit since the Mott term is of order $\hbar^2$. It is clear that only scatterings in the nearly forward direction contributes to this limit, i.e., the momentum transfer $\hbar \underset{\sim}{q} \rightarrow 0$. The collision integral (3), however, is logarithmically divergent at large q (i.e. close collisions). As pointed out by the study of Wyld and Pines[10], an alternative classical limit of the quantum-mechanical collision integral can be taken which preserves the role of finite momentum transfers and avoids convergence difficulties at large q, at the expense, however, of divergent behavior at small q (distant collisions).

Specifically, the substitution $\frac{\hbar}{m}\underset{\sim}{q} \equiv \underset{\sim}{u}$ casts (14) into the form

$$\left(\frac{\partial \tilde{f}}{\partial t}\right)_{\text{Coll.}} = -\frac{4ne^4}{m}\int d^3v' \int d^3u \left\{ \frac{1}{u^4}\left|\tilde{K}\left(\frac{m\underset{\sim}{u}}{\hbar}, \frac{1}{\hbar}\left(\tfrac{1}{2}m(\underset{\sim}{v}+\underset{\sim}{u})^2 - \tfrac{1}{2}mv^2\right)\right)\right|^{-2} \right.$$
$$\left. - \frac{1}{2u^2(\underset{\sim}{v}-\underset{\sim}{v}'+\underset{\sim}{u})^2} \mathrm{Re}\left(\left[\tilde{K}\left(\frac{m\underset{\sim}{u}}{\hbar}, \frac{1}{\hbar}\left(\tfrac{1}{2}m(\underset{\sim}{v}+\underset{\sim}{u})^2 - \tfrac{1}{2}mv^2\right)\right)\right]^{-1}\right)\right\}$$
$$\times\, \delta\left[\tfrac{1}{2}m(\underset{\sim}{v}+\underset{\sim}{u})^2 + \tfrac{1}{2}m(\underset{\sim}{v}'-\underset{\sim}{u})^2 - \tfrac{1}{2}mv^2 - \tfrac{1}{2}mv'^2\right]\left[\tilde{f}(\underset{\sim}{v})\tilde{f}(\underset{\sim}{v}') - \tilde{f}(\underset{\sim}{v}+\underset{\sim}{u})\tilde{f}(\underset{\sim}{v}'-\underset{\sim}{u})\right] \qquad (15)$$

In the limit $\hbar \rightarrow 0$, all that happens now is $\tilde{K} \rightarrow 1$ so that (15) goes over into the ordinary Boltzmann collision integral appropriate to the Mott scattering cross-section. We are thus led to the conclusion that the new collision integral will lead to an alteration of the cut-off procedure usually applied to (3) at large q. In particular, we note that as $u \rightarrow \infty$, the integrand of (15) approaches half its ordinary value, corresponding to the fact that the Pauli principle inhibits close encounters between electrons of parallel spin.

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